Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 153 °C

Global applicability domain: Inside

Local applicability domain index: 4.05e-01

Confidence level: 3.75e-01

Nearest Neighbors from the Training Set

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Bentazone
Measured: 138
Predicted: 153

Image not found

Diazoxide
Measured: 331
Predicted: 297

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5-Dimethylaminonaphthalene-1-sulfonamide
Measured: 220
Predicted: 224

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Nimesulide
Measured: 144
Predicted: 160

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Chloroxuron
Measured: 151
Predicted: 144